Diffuse X-Ray Scattering Study of the Local Atomic Order and Pair Displacements in a $Au_{50}Cu_{50}$

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Earlier diffuse x-ray scattering measurements on Au Cu_3 alloy[1] with a single x-ray energy concluded that Au-Au first neighbor pairs are on average closer together than Au-Cu or Cu-Cu pairs. This conclusion is contrary to intuition as the Au atom is ~13% larger then the FCC Cu lattice and cast doubt on the sensitivity of diffuse x-ray scattering to measure atom size. Also, the addition of Au to Cu expands the lattice and ordering of $AuCu_3$ (which makes more Au-Cu first neighbor pairs) decrease the lattice parameter. Theoretical considerations and EXAFS measurements support the notion of larger Au-Au and smaller Cu-Cu first neighbor bond distances. Because of our advancements in the use of energy tunable synchrotron radiation to highlight specific elements in diffuse x-ray scattering measurements and to separate the individual specific pair bond distances, we undertook these measurements to show their application to a wide variety of solid solutions with atomic numbered elements both close and widely separated.[2-6]

Three dimensional volume measurements with x-ray energies chosen to be 20 eV below the Cu K edge and Au L_3 edge and an energy in-between reveal the asymmetry in the short-range order maxima associated with the variations in the neighboring atom bond distances. Diffuse x-ray data for a plane in reciprocal space is shown in Figure 1. Analysis is underway to recover the individual pair displacements.

References

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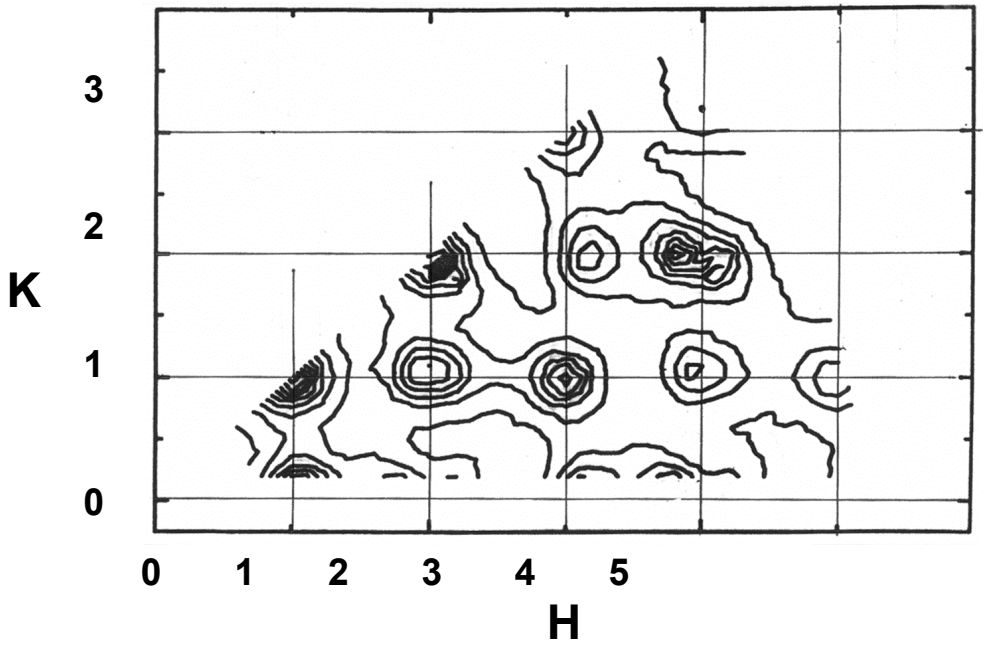

Figure 1. A planer cut through reciprocal space at L=0.2 for a $Au_{50}Cu_{50}$ single crystal quenched from 475ºC. At the x-ray energy of 8.964 keV, the maximum contrast between Au and Cu atoms is obtained. The short-range order maxima [near (2,1), (3,1), (4,1), (3,2), (3,3)] show a systematic displacement (asymmetry) associated with the different atom pair bond distances.